DIMERIZATION ENERGETICS OF DNA MINOR GROOVE BINDERS

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The energy analysis of a dimerization in aqueous solutions of seven biologically active lexitropsins, which are different by structure, was carried out with the use of the molecular simulation method. The main stabilization of dimers was shown to take place owing to hydrophobic and intermolecular van der Waals interactions. The latter are mainly associated with energy-favorable contacts between the aromatic rings of molecules and their peptide groups. Despite the significant dipole moments of the molecules concerned, the electrostatic interactions are relatively weak and destabilize the complexes because of the unfavorable relative arrangement of molecular dipoles. Entropic factors and the dehydration were shown to also hinder the dimerization.